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RELEVANT CITATIONS:

Peter, Katherine T., et al. "Nontargeted Analysis Study Reporting Tool: A Framework to Improve Research Transparency and Reproducibility." *Analytical Chemistry* 93.41 (2021): 13870-13879. DOI: 10.1021/acs.analchem.1c02621

BP4NTA (2022): NTA Study Reporting Tool (PDF). figshare. DOI: 10.6084/m9.figshare.19763482

BP4NTA (2022): NTA Study Reporting Tool (Excel). figshare. DOI: 10.6084/m9.figshare.19763503

BP4NTA
BENCHMARKING AND PUBLICATIONS FOR NON-TARGETED ANALYSIS

NTA Study Reporting Tool

Please read before using!

Purpose: This Tool was developed for use by NTA researchers and reviewers to assess the quality of NTA study reporting, and the resulting scores reflect solely whether the reporting is sufficiently complete and transparent (based on current, best available understanding of the environmental, food, and exposomics NTA communities). The Tool is not intended for evaluation of the quality of the study or resulting data.

We also encourage two supplementary uses of the Tool: 1) to guide study design - by considering what should be reported, a researcher is inherently encouraged to incorporate the necessary aspects into their study design, and 2) as a starting point for (or portal to) relevant reference content and resources, which are available via the BP4NTA website (www.nontargetedanalysis.org).

Notes & Guidance: The "Example Information to Report" column provides a brief list of representative items relevant to each sub-category - not all are required or necessary for every study. Researchers and reviewers should use their expertise and discretion to determine which points pertain to a given study, and whether additional details not explicitly listed are also critical to report. Additionally, certain sub-categories may not be relevant to a given study (hence the option to select "NA"), or may be less critical to the overall quality and completeness of reporting. To evaluate these aspects, we strongly encourage users to both consider the study type and objectives (e.g., method development, performance evaluation, field application), as well as conceptual linkages across subcategories (e.g., between Statistical Analysis and Statistical Outputs).

Please also note that the Sections (Methods and Results) are not intended to indicate the location in a manuscript where the information is reported - a user should consider the manuscript in its entirety (including any supporting documents and/or citations). We also encourage reviewers to include a rationale, so that authors/researchers may readily address concerns.

Scoring: *NA* = not applicable (gray); *3* (blue) is the highest score and *0* (red) is the lowest. See scoring system explanation provided below.

✔ **Toggle to show score colors vs. fillable fields**

Section	Category	Sub-Category	Example Information to Report	Score (drop-down menu) NA 0 1 2 3	Rationale for score
Methods	Study Design	Objectives & Scope	• Study goals and hypotheses • Scope of the study with respect to use of NTA / suspect screening • Expected chemical coverage of approach and potential limitations		
		Sample Information & Preparation	• Sample collection/replication, handling/storage, preparation, extraction, & clean-up methods (and related QA practices) • Intended use of samples (e.g., method development, compound identification, etc.) • Development and intended use of blanks		
		QC Spikes & Samples	• Development of QC spikes/samples (e.g., isotopically labeled standards/spikes, native standard spikes, matrix pools) • Intended use of QC spikes/samples (e.g., to monitor instrument performance, data normalization, etc.)		
	Data Acquisition	Analytical Sequence	• Sample randomization and use of replicate injections • Inclusion of blanks and QC samples in the acquisition sequence • Information about single vs. multiple analytical batches		
		Chromatography	• Instrument specifications • Method settings (e.g., column/guard, mobile phases, gradient, injection techniques)		
		Mass Spectrometry	• Instrument specifications • Instrument calibration and/or tuning procedures • Method settings (e.g., acquisition parameters, such as polarity, resolution, data-dependent vs. data-independent)		
	Data Processing & Analysis	Data Processing	• File conversion information (e.g., to open-source format, centroiding) • Software program(s) used • Workflow steps (e.g., peak picking, RT calibration, alignment, gap filling) and settings • Feature detection thresholds (e.g., replicate detection criteria; min height, area, or S/N levels; comparison to occurrence/abundance in blanks) • Data correction or normalization methods (e.g., peak area/height normalization or scaling, blank subtraction)		
		Statistical & Chemometric Analysis	• Software programs(s)/package(s) used & samples/sample groups to which analyses were applied • Basic statistical analysis method goals (e.g., summarize data, evaluate variability, hypothesis testing), type (e.g., Wilcoxon rank sum test, Chi-square test), assumptions, and settings/thresholds • Chemometric analysis method goals (e.g., prioritize features, compare/classify samples, evaluate relationships between features), type (e.g., differential analysis, hierarchical clustering, dimensionality reduction), assumptions, and settings/thresholds		
		Annotation & Identification	• Software program(s) used (or description of manual annotation/identification efforts) • Libraries and databases used (including details such as chemical coverage, resolution, metadata inclusion; information about in-house databases) • Workflow steps (e.g., formula assignment, suspect screening, MS/MS spectral interpretation or library matching) • Workflow methods & settings (e.g., formula prediction method, scoring algorithms; mass error/RT tolerances, accepted match scores)		
Results	Data Outputs	Statistical & Chemometric Outputs	• Basic statistical outputs (e.g., adj. p-values, standard deviations, test statistics) • Results of chemometric analyses (e.g., reported classifications/groupings of features or samples, observed trends in the data) • Visuals/plots (e.g., Venn diagrams, heatmaps, clustering dendrograms, volcano plots, network diagrams, PCA and loading plots) • New statistical metrics, algorithms, packages, and/or scripts		
		Identification & Confidence Levels	• Reported identifications and associated confidence levels (e.g., levels described by Schymanski et al., *ES&T*, 2014) • Supporting data for annotation/identification (e.g., formula match scores, fine isotope pattern, retention time match, MS/MS match scores, source of MS/MS spectra) • For features with lower confidence IDs, (i.e., not standard-confirmed), proposed tentative structures and other annotated data • Semi-quantification or quantification data • Exported MS/MS spectra (e.g., as a library, database, or deposition into online repository)		
	QA/QC Metrics	Data Acquisition QA/QC	• Quality: Adherence to QA/QC protocols for sample preparation and data acquisition • Boundary: Description of the potential impacts of methods (sample prep, chromatographic, MS) on observable chemical space • Accuracy: Reported chromatographic and mass accuracy • Precision: Variability of observed retention time, precursor mass error, and abundance		
		Data Processing & Analysis QA/QC	• Quality: Outcomes of QC checks along the data processing & analysis workflow • Boundary: Impact of data processing & analysis method(s) on observed chemical space, observed limits of detection/ID • Accuracy: Performance measures (True Positive Rate, False Positive Rate, etc.) for known compounds or samples with known classification • Precision: Reproducibility/repeatability of performance measures for known compounds or samples with known classification; Calculations such as False Discovery Rate, F1 score, etc.		

Scoring System Explanation

0	No elements of relevant reporting are present.	**1**	Some elements of relevant reporting are present, but major improvements are needed.	**2**	Most elements of relevant reporting are present, but minor improvements are needed.	**3**	All elements of relevant reporting are present.	**NA**	Reporting not relevant to the study.